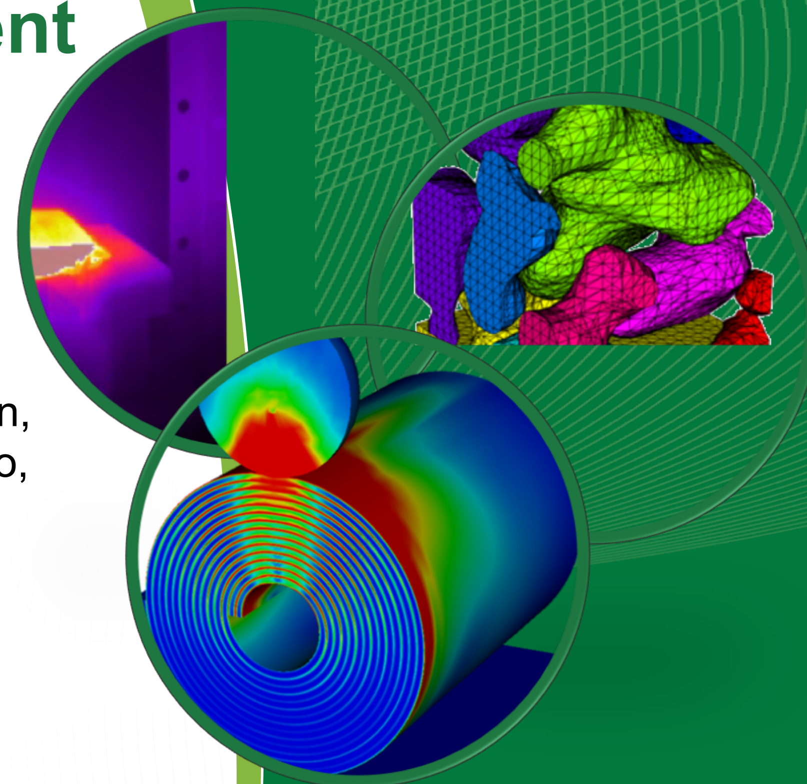
Enhancement and Deployment of VIBE, the Open Architecture Software (OAS) Environment



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2018 U.S. DOE Vehicle Technologies Office Annual Merit Review

June 20, 2018 **Project ID:** bat300

CABS Consortium for Advanced Battery Simulation

Oak Ridge National Laboratory
Argonne National Laboratory
Berkeley Lab
Sandia National Laboratories

Overview

Timeline

- Start
  - October 2015
- Finish
  - September 2018
- Percent complete: 55%

Barriers Addressed

C. Performance
D. Abuse Tolerance, Reliability, and Ruggedness
E. Life

Budget

- FY17
  - Total CABS Funding: 2,225K
  - This effort: 570K
- FY17
  - Total CABS Funding: 1,398K
  - This effort: 440K

Partners

- LBNL
- SNL
- ANL
- as well as the NREL-led CAEBAT project team

Relevance and Project Objectives

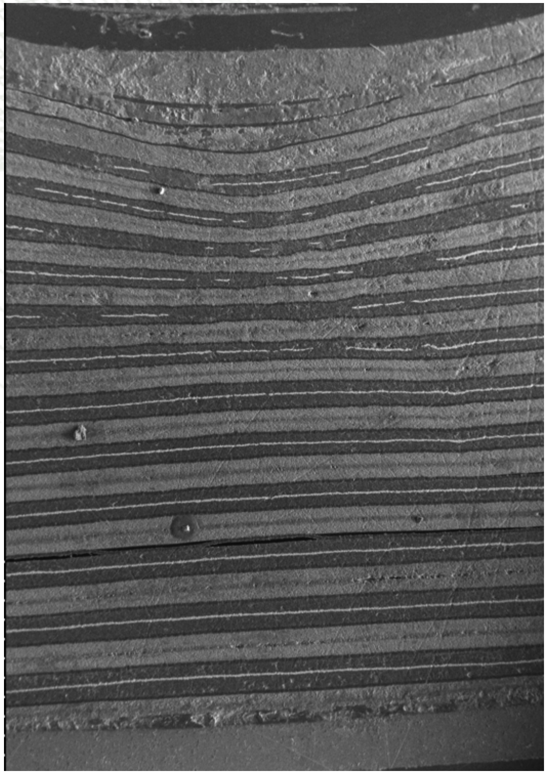
- Major barriers for increasing battery energy density and power, increasing safety and reducing cost include
  1. insufficient understanding of the underlying physical phenomena that limit battery performance and safety
  2. lack of validated predictive simulation tools.

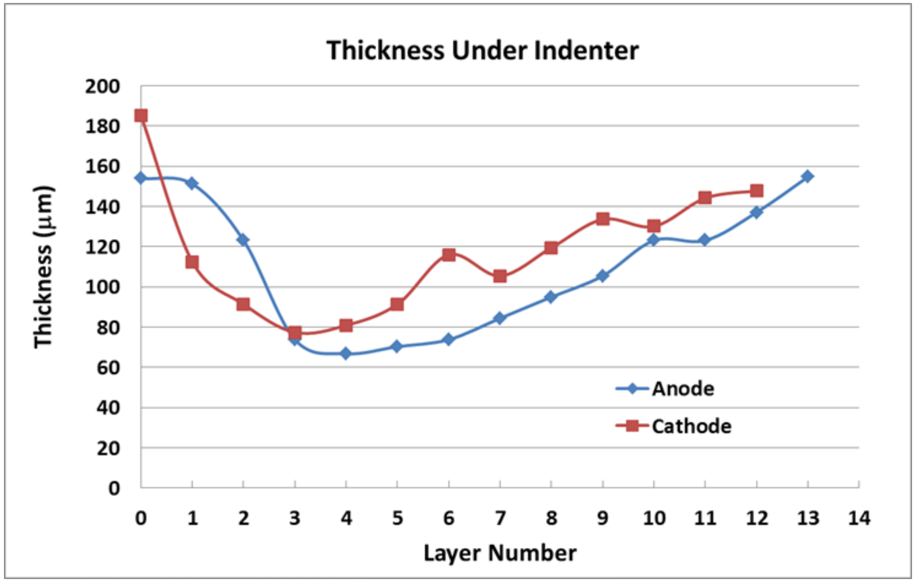
- CABS is addressing (1) by developing new experiments for properties with largest uncertainties and developing new validated models that allow researchers to explore battery response under both normal and abusive conditions, and is addressing (2) by deploying increasingly capable and computationally efficient releases of the Open Architecture Software (OAS) and components of the Virtual Integrated Battery Environment (VIBE), developed as part of CAEBAT.

Milestones (FY17)

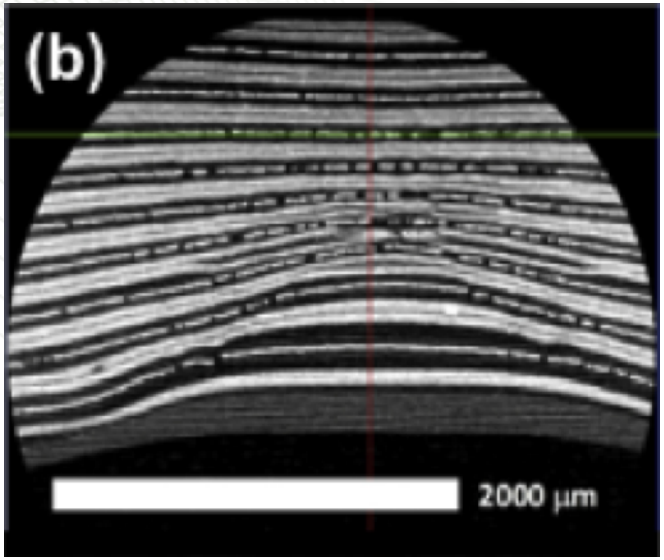
IDs indicate whether milestones are primarily experimental (E), computational (C), or integrated (I).							
ID	FY17	Lead	Q1	Q2	Q3	Q4	Status
I.3	Demonstration of ability to construct 3D meshes of electrodes using reconstructions from micro-tomography	SNL	P				Complete
E.3	Potential-dependent solid diffusivities for Li-ion and EIS	LBNL		P			Complete
I.4	Demonstrated ability of VIBE/OAS to simulate onset of short-circuit due to mechanical abuse informed by microstructure	ORNL		D			Complete
E.4	Data from mechanical deformation tests	ORNL			P		Complete
C.2	Validated constitutive models and failure criteria for electrode materials and spirally wound, wound prismatic, and stacked electrodes under indentation	ORNL				P	Complete
I.5	Deployment of VIBE/OAS with integrated multiscale capability	ORNL				S	Complete

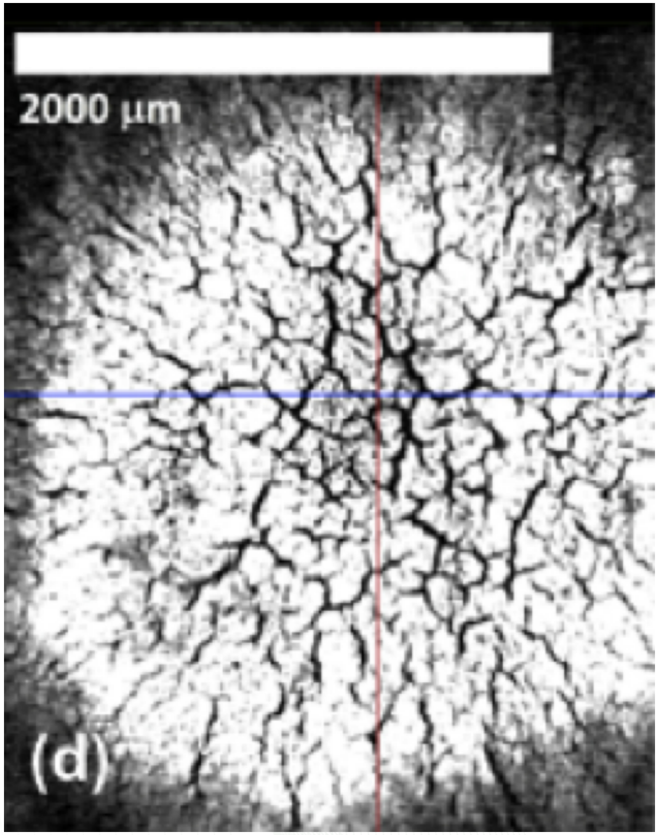
Approach : SEM cross sections of deformed cells





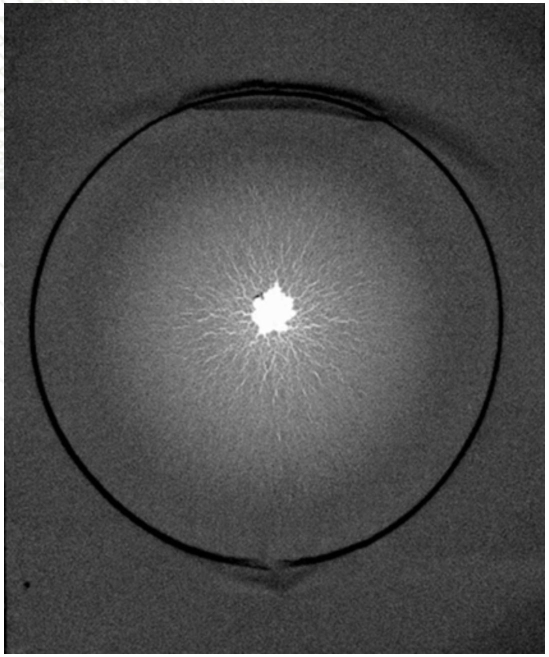
Approach : Fragmentation of anode (Copper) current collectors

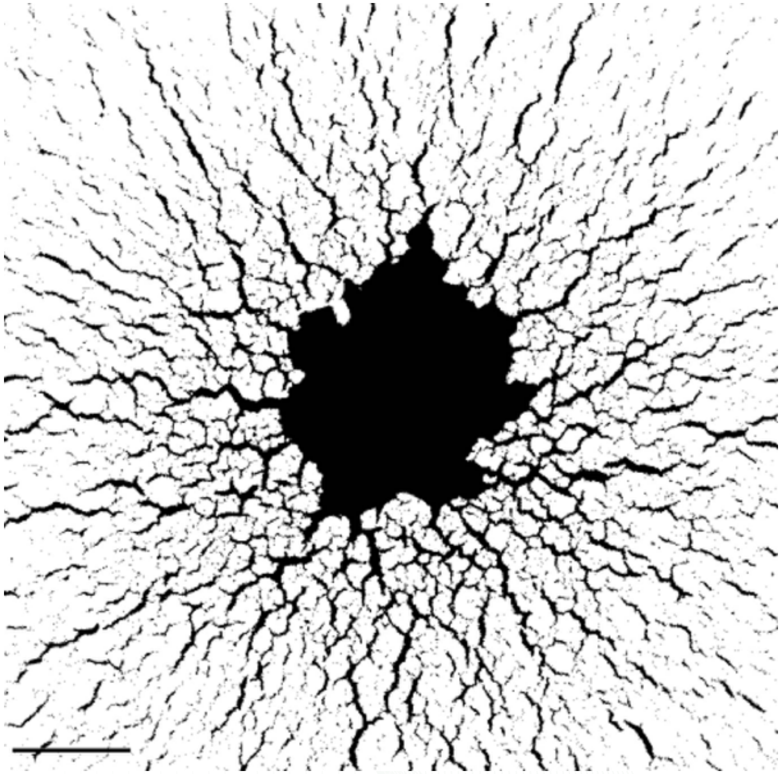




X-ray tomographic of cross-section and in-plane section

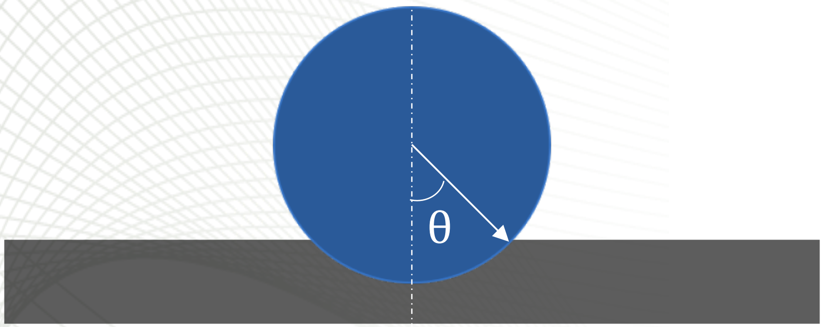
Approach : Fragmentation of anode (Copper) current collectors





X-ray radiographs showing 'mud cracks' of single layer of anode

Approach: Reconstructing the area of fragmentation and problem setup

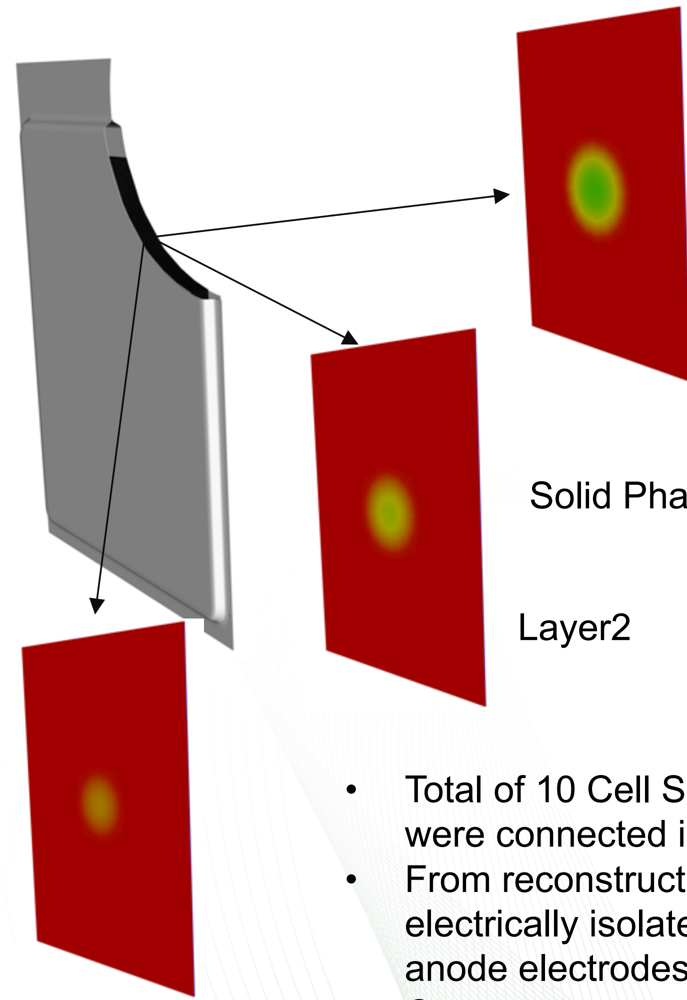


Indenter diameter ~ 12.7 mm
Deformation ~ 55% of thickness
Cell dimensions: 40mm x 30mm x 4.5mm

$$\theta = \cos^{-1}\left(\frac{3.85}{6.35}\right) \approx 52.67°$$

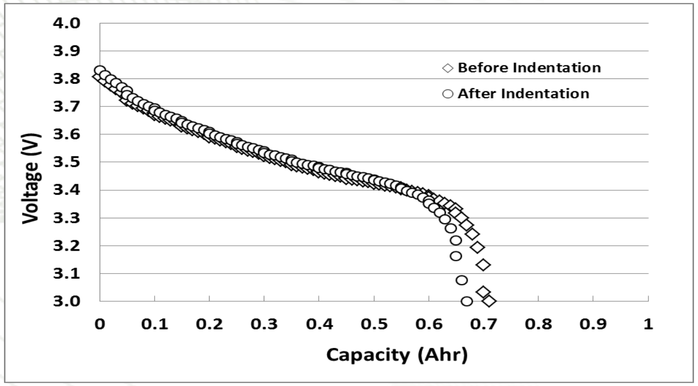
Assuming symmetric indentation, length of contact(/fragmentation) is estimated to be

layer 1 ≈ 11.63 mm
layer 2 ≈ 10.33 mm
layer 3 ≈ 9.00 mm
:

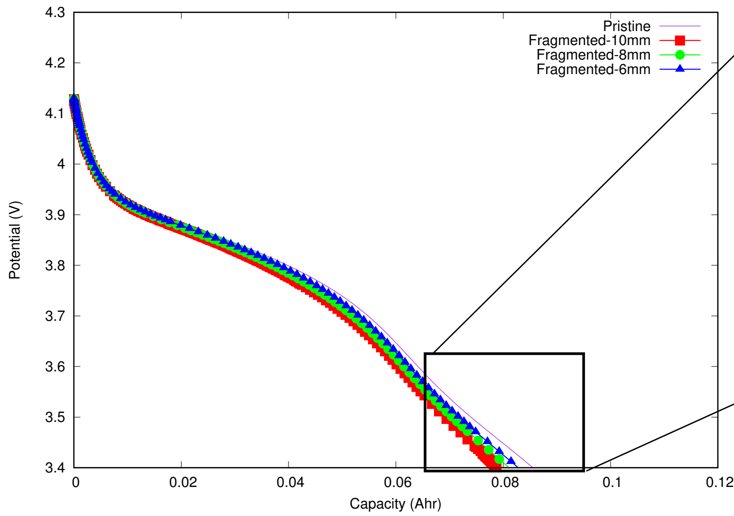


- Total of 10 Cell Sandwich layers were connected in parallel
- From reconstruction we have electrically isolated the first five anode electrodes
- Constant current discharge is imposed at 1C rate

Technical Accomplishment : Total extracted capacity of deformed cell

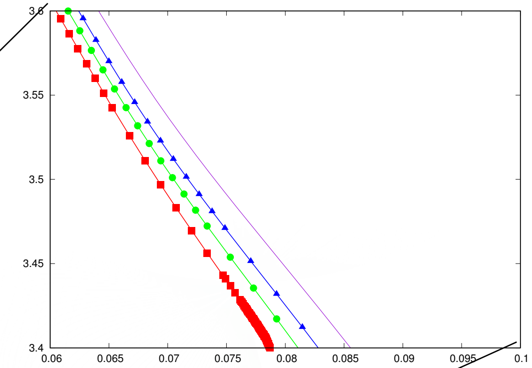


Experiment



Simulation

Total Capacity extracted from deformed cell of 10 layers: 97.63%



Anode Layer	Isolated circle dia.	Extracted Capacity %
Layer 1	10 mm	90.5%
Layer 2	8 mm	94.1%
Layer 3	6 mm	96.7%

Summary Milestone-I.4 (Status: Complete)

Goals

- Conduct microstructure simulations
  - Upscaling effective transport properties
- Capability to simulate Onset of electrical short
  - Coupled Mechanical-electrochemical-thermal simulations
- Design experiments to generate validation data

Approach / Strategy

- Estimate appropriate binder location
- Upscale properties at varying pressures
- Simulate short from mechanical induced deformations

Results

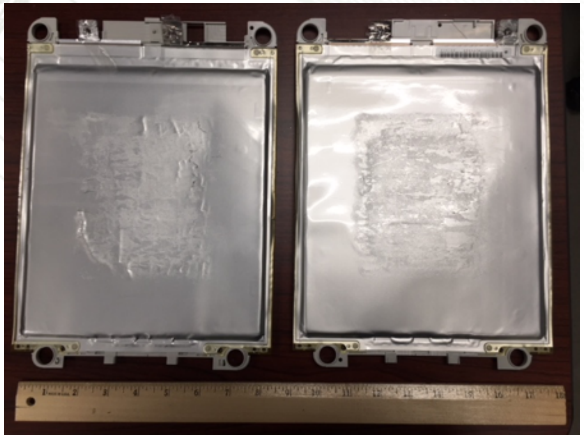
- Separator failure criterion and effective contact area dictates the severity of short
- Microstructure reorganization under mechanical loading influences the effective transport properties.
- Copper foil fragmentation electrically isolates the electrode leading to lower extracted capacity of deformed cells

Milestones (FY18)

IDs indicate whether milestones are primarily experimental (E), computational (C), or integrated (I).							
ID	FY18	Lead	Q1	Q2	Q3	Q4	Status
C.3	Coupled thermo-electro-mechanical microstructure simulations of overcharge and mechanical abuse scenarios	SNL	P				Ongoing
E.5	Obtain electrode image data from cycled electrode material	LBNL	P				Ongoing
C.4	Demonstrated mesoscale simulations	ORNL		P			Ongoing
C.5	Demonstrate improved computational efficiency on a benchmark pack-level simulation using a hierarchy of electrochemical models for US06 drive	ORNL			P		Ongoing
C.6	Validated constitutive models & failure criteria for electrode materials & spirally wound, wound prismatic, & stacked electrodes under bending for pouch cell	ORNL				P	Ongoing
I.5	*Deployment of VIBE/OAS with efficient, validated mechanistic models*	*ORNL*				S	*Ongoing*

Approach: 2013 Nissan Leaf battery cell and test equipment

- Charge and discharge tests performed on single battery cell
- Hybrid Performance Pulse Characterization (HPPC) test also performed

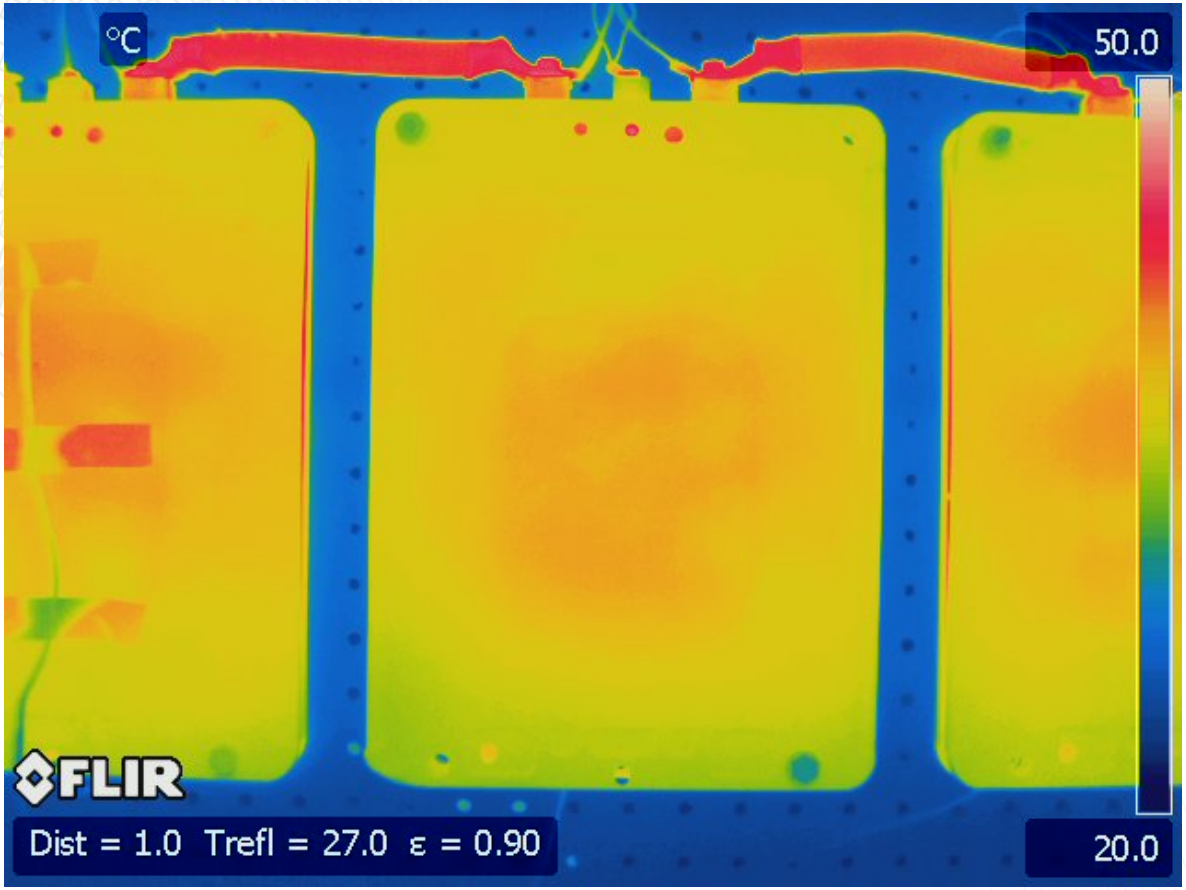


Battery cell from disassembled Nissan Leaf module. Battery pack provided by NREL.

Battery cell specs	
Cell type	laminate
Cathode material	$LiMn_2O_4$ with $LiNiO_2$
Anode material	graphite
Rated capacity (0.3C)	33.1 Ah
Average voltage	3.8 V
Length	11.417 in (290 mm)
Width	8.504 in (216 mm)
Thickness	0.2795 in (7.1 mm)
Weight	1.7624 lbs (799 g)

CSZ chamber (left) and Bitrode MCV cycler (right) for charge/discharge and HPPC battery cell tests at ORNL. Cycler has 8 channels where each channel has max current of 25 A.

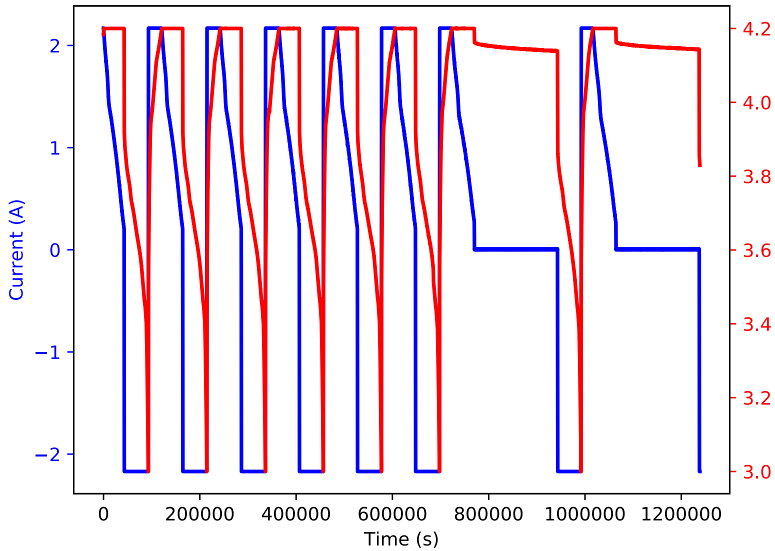
Approach: Experimental data from NREL (Kandler/Hsin)



- Thermal IR movie of Nissan Leaf module at US06 drive cycle
- Adjacent modules are connected with busbars where considerable heating is taking place.
- Processing data to isolate the center module to understand the effects of cycling protocol

Approach: Charge and discharge cycling tests

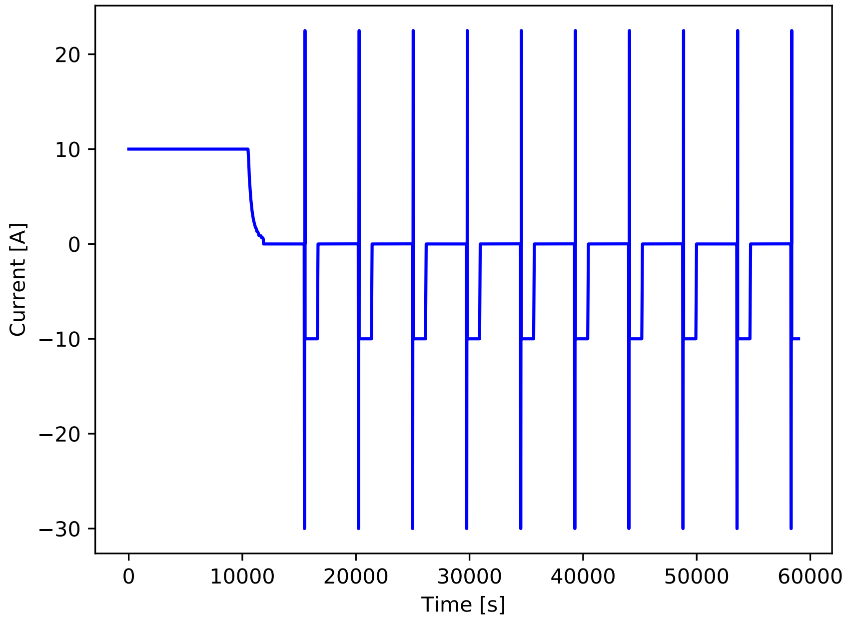
- Charge/discharge cycles performed at ambient temps. of 10°C, 24°C, and 40°C
- Cycle test procedure
  – 5 min rest
  – C/15 discharge to 3.0 V
  – 5 min rest
  – C/15 constant current charge to 4.2 V and constant voltage charge at 4.2 V until the current is < 10% of C/15
  – Repeat above steps for each temperature cycle

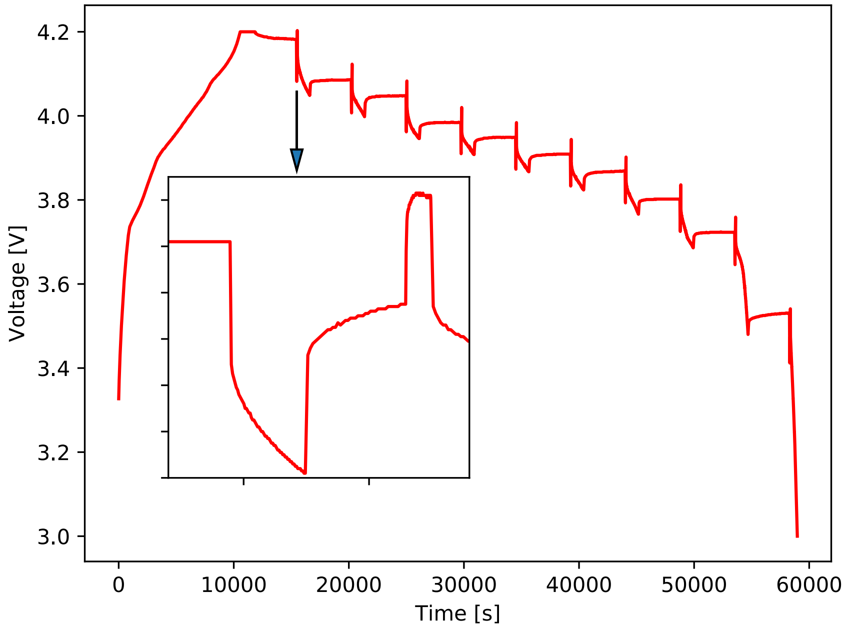


Charge and discharge cycles of Nissan Leaf battery where each cycle was performed at a different ambient temperature. Source: test data from Hsin Wang at ORNL.

Approach : Hybrid Performance Pulse Characterization (HPPC) tests

- Low current HPPC tests conducted at 10°C, 25°C, and 40°C
- Discharge pulses at 10% SOC





Approach : Develop EC circuit model from HPPC battery cell data

$$\frac{dz}{dt} = -i(t)\eta(t)/Q$$

$$\frac{di_{R_1}(t)}{dt} = -\frac{1}{R_1C_1}i_{R_1}(t) + \frac{1}{R_1C_1}i(t)$$

$$v(t) = OCV(z(t)) - R_1\, i_{R_1}(t) - R_0\, i(t)$$

z = state of charge (SOC)

i = current in the cell

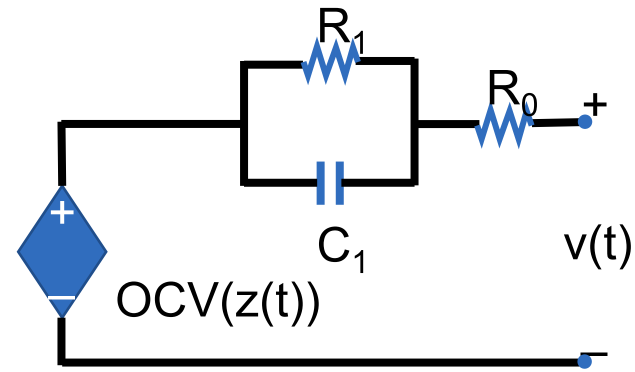
Q = total capacity of the cell

OCV = open circuit voltage

R_1, C_1 = parallel resistor-capacitor circuit

R_0 = equivalent series resistance

i_{R1} = current thru R_1 branch of R-C circuit



Equivalent circuit model for the Nissan Leaf battery cell represented by a series resistance (R_0) and a parallel RC pair (R_1, C_1).

Approach : Current through the R_1 branch

$$\frac{di_{R_1}(t)}{dt} = -\frac{1}{R_1C_1} i_{R_1}(t) + \frac{1}{R_1C_1} i(t)$$

$$i_{R_1}[k+1] = exp\left(-\frac{\Delta t}{R_1C_1}\right) i_{R_1}[k] + \left(1 - exp\left(-\frac{\Delta t}{R_1C_1}\right)\right) i[k]$$

where
i = current
i_{R1} = current through R_1 resistor
k = time step

Current through R_1 and C_1 must be equal to i(t).

Assume i_{R1} is zero at initial time step k=0 since i[0]=0.

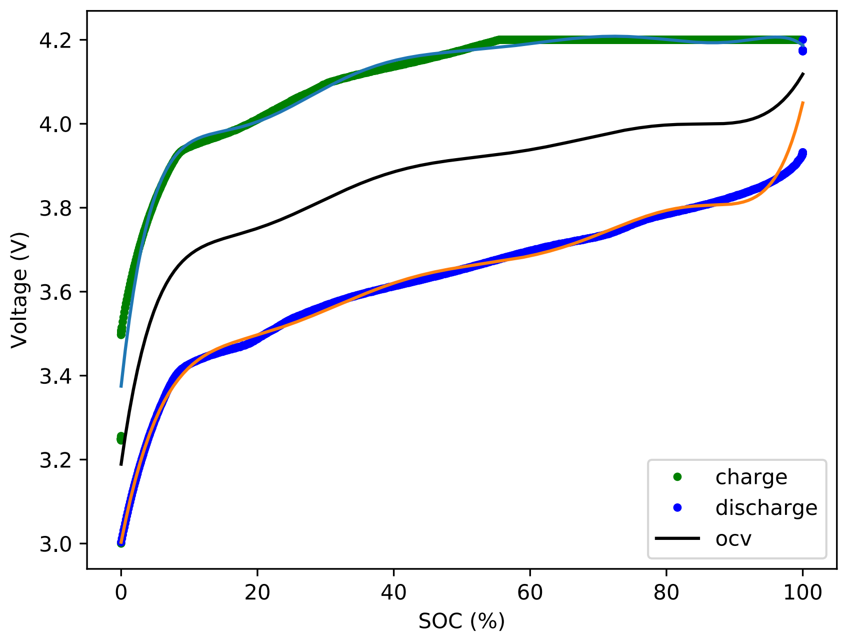
Open-circuit voltage (OCV) from charge/discharge tests

- Least-squares polynomial fit of charge and discharge data

$$p(x) = c_0 + c_1\,x + \ldots + c_n\,x^n$$

- OCV as the average of the charge and discharge curves
- OCV can be linearly interpolated at intermediate SOC

$$v(t) = \underbrace{OCV(z(t))}_{\Uparrow} - R_1\,i_{R_1}(t) - R_0\,i(t)$$

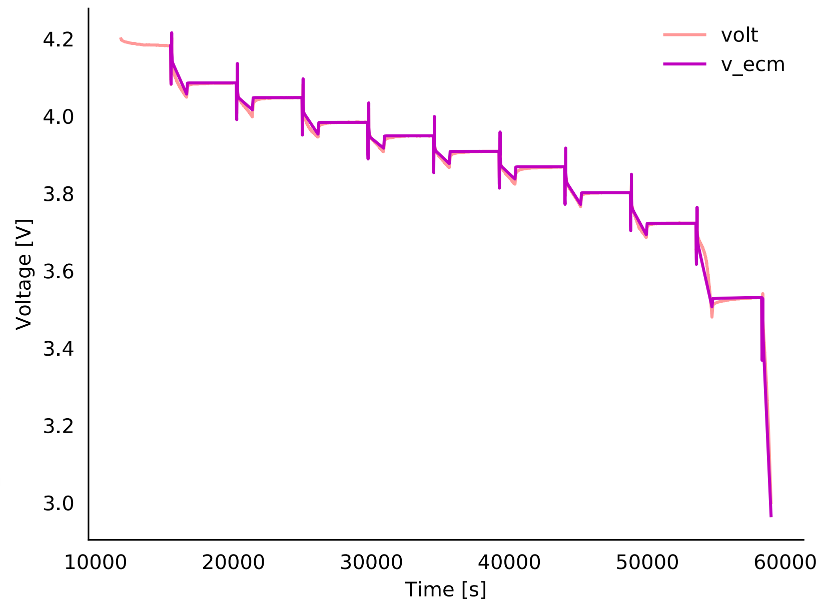


Technical Accomplishment : Comparison of lower order circuit model to HPPC voltage profile

- A single RC pair is sufficient to capture HPPC voltage profile of the Nissan Leaf battery cell

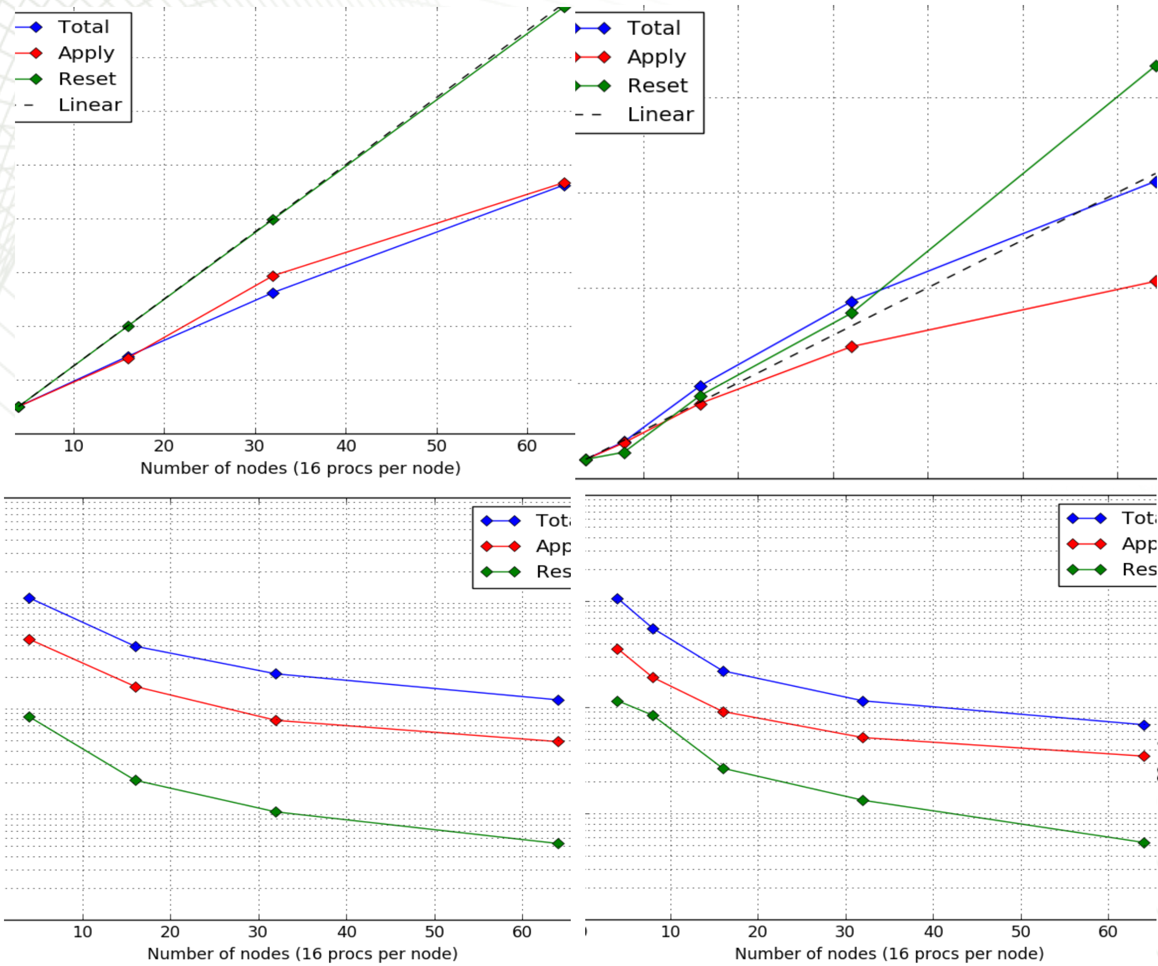
V_{max} = 4.203 V
V_{min} = 3.0 V
I_{max} = 22.5 A
I_{min} = -30.0 A

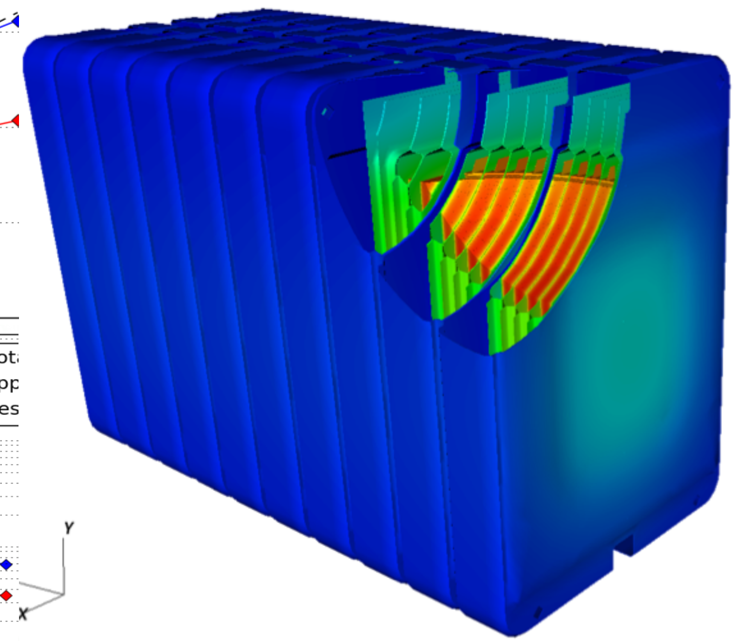
Q = 32.0 Ah
SOC_{max} = 100.00 %
SOC_{min} = 0.05 %
RMSE = 0.02057



Comparison of HPPC voltage profile (volt) with ECM voltage (v_ecm). Model uses a single RC parallel circuit with a resistor in series.

Technical Accomplishment : Improved performance of the coupled lower order electrochemical and thermal transport AMPERES





CABS Consortium for Advanced Battery Simulation

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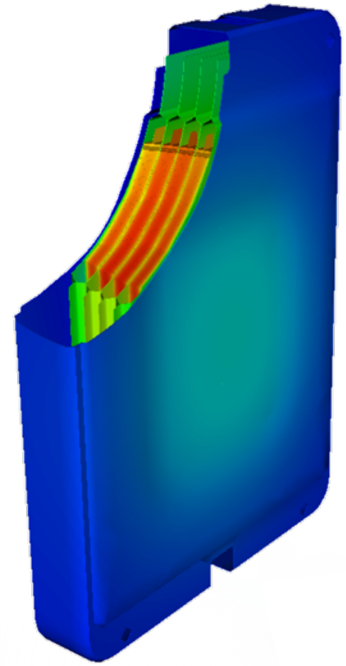
Sandia National Laboratories

Summary Milestone-C.5 (Status: Complete)

Goals

- Software design updates to improve VIBE computational performance
  - Continuous execution of physics based solver components
- Capability to simulate dynamic discharge
  - Coupled electrochemical-thermal simulations under variable potentio-static / galvano-static conditions
- Deployment of the software



Approach / Strategy

- Launch component as daemon
- Python component wrapper translates calls from simulation driver into messages to daemon
- Deployment via docker container

Results

- The new release of software has reduced the simulation time by 50%.
- New test case of coupled simulation for hybrid pulse power characterization of the battery module.

Responses to Previous Year Reviewers' Comments

AMR 2017 Review Comments	Response
"The reviewer will assume it is all explicit FEA. The reviewer saw a LS-Dyna simulation in slides and questioned if the understood approach is to develop a python wrapper to launch the FEA codes. "	The OAS/VIBE python framework does limit the time-stepping schemes that can be used in the underlying physics components that are coupled. Since for the mechanics component LS-Dyna software is employed, the python wrapper for the current simulation uses explicit scheme where exchange of battery state data.
"upscaling effective properties from microstructure simulation the reviewer did not see the effects of temperature being considered."	No. The temperature effects are considered secondary for upscaling the effective electronic transport properties.
"the different types of simulations were not specified…The reviewer said that it seems hard to believe that an explicit heat transfer model is the bottleneck in the simulation. The reviewer saw that the electrical model is actually the limiting case. "	The simulation capabilities are specified in the recap slide. The reviewer is right in noting that thermal transport is not the limiting step in the process instead it is mechanical and electrochemical transport. To address these issues we used explicit FEA and also developing lower order electro chemical models.

Responses to Previous Year Reviewers' Comments

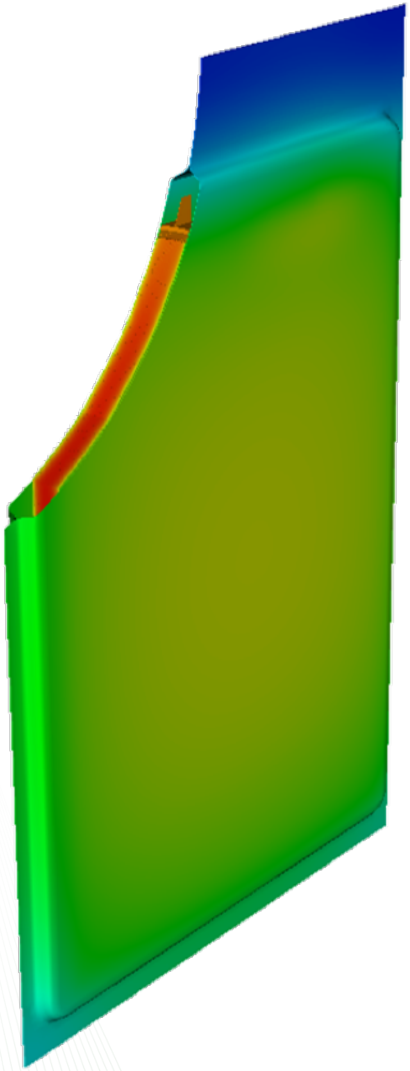
AMR 2017 Review Comments	Response
"The reviewer said that the milestone on shorts seems like a good goal but it is not clear how well it simulates real data."	As reviewer noted shorting of the cell is a complex process and team is trying to understand the failure mechanisms of different components in incremental steps. The goal of the effort is to identify the critical step in event of the mechanical crush of batteries.
"The reviewer asked does the proposed understanding of the influence of temperature variations during dynamic discharge of battery module cover automotive battery working range."	Yes. The testing protocol US06 used by the regulators/industry to measure performance of the batteries are used to understand the temperature variations during dynamic discharge.
"The reviewer said that it would also be worthwhile to maybe write a python graphical user interface (GUI) to run these simulation and culminate results…also said it would be nice to see more details on message passing, sockets or files. The reviewer asked if the PI has the source to these FEA codes"	The PI's will discuss options to consider the reviewer's suggestion. No, we do not have source to proprietary code owned by the commercial entities. The OAS/VIBE provide a python based API's to couple between various software.

Collaboration and Coordination with Other Institutions

- Collaboration with SNL (CABS sub) to bring microstructure modeling capabilities into VIBE/OAS
- Collaboration with LBNL/ANL (CABS sub) to refine tomography imaging data for simulations
- Monthly testing user group meeting with NREL to exchange experimental data for validation of dynamic discharge of battery module
- Collaboration with FORD (Prime) to develop multi-physics simulation tool to predict response under mechanical impact in LS-Dyna
- Active project with NHTSA on characterization experiments and simulations to develop crashworthiness models.

Remaining Challenges and Barriers

- Binder distribution and adhesion to the electrode particles
  - binder resolution with tomography imaging
  - bonding strength between binder/electrode particles
- Predicting the critical temperature threshold leading to thermal runaway
  - insufficient understanding of complete chemical mechanisms during runaway
- Electrochemical cycling of the NMC/Graphite electrodes under deformed configurations
  - uncontrolled experiments could lead to internal-short due to Li plating



Any proposed future work is subject to change based on funding levels

Proposed Future Research

- Reduced order modeling of dynamic discharge profiles.
- Understanding the influence of temperature variations during US06 dynamic discharge causing SOC non-uniformity in battery module
- Upscale effective properties under varying porosities and binder re-allocation
- Complete integration of microstructure models from SNL into VIBE/OAS
- Implement closure models from surface energy characterization to predict slip bands at the electrode scale

Any proposed future work is subject to change based on funding levels

Summary

Objectives

- Software design updates to improve VIBE computational performance
- Capability to simulate dynamic discharge
- Conduct micro-structure simulations to upscale effective transport properties
- Capability to simulate onset of electrical short using coupled mechanical-electrochemical-thermal simulations

Approach

- Launch component as daemon for continuous execution of physics based solver
- Python component wrapper translates calls from driver into messages to daemon
- Estimate appropriate binder location
- Upscale properties at varying pressures
- Simulate short from mechanical induced deformations

Accomplishments and progress

- New release of VIBE has reduced the simulation time by 50%.
- Algorithmic and software design improvements that allows for seamless integration and deployment via docker container
- Implemented variable potentio-static, galvano-static and open circuit voltage(OCV) resting conditions
- Separator failure criterion and effective contact area dictates the severity of internal short
- Microstructure reorganization under mechanical compression influences the effective transport properties during onset of short.

Future work

- Understanding the influence of temperature variations during dynamic discharge of battery module
- Implement closure models from surface energy characterization to predict slip bands at the electrode scale

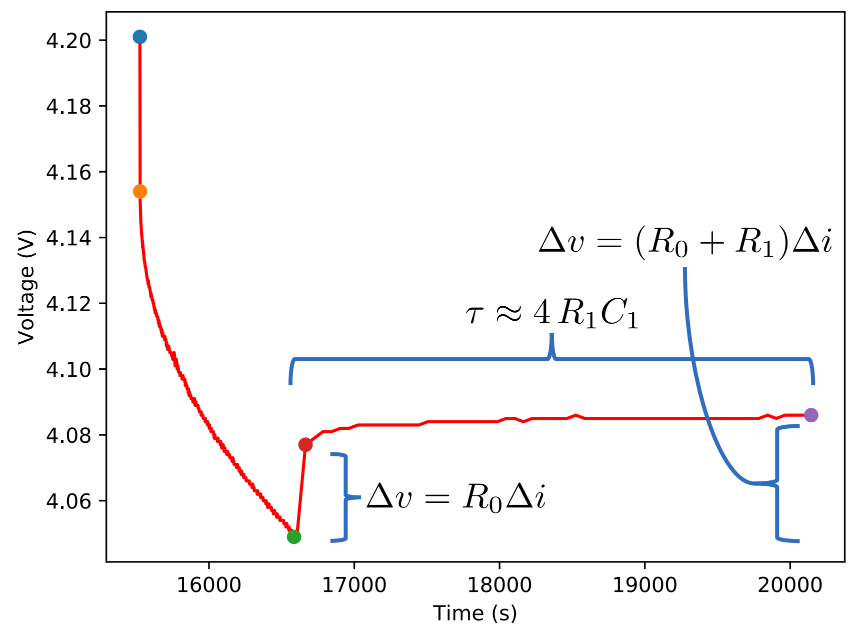
Technical Back-Up Slides

Determine R-C parameters from HPPC tests

- Resistor and capacitor parameters determined from HPPC tests
- Parameters calculated from HPPC voltage profile for each 10% change in SOC

$$\frac{di_{R_1}(t)}{dt} = -\frac{1}{R_1 C_1} i_{R_1}(t) + \frac{1}{R_1 C_1} i(t)$$

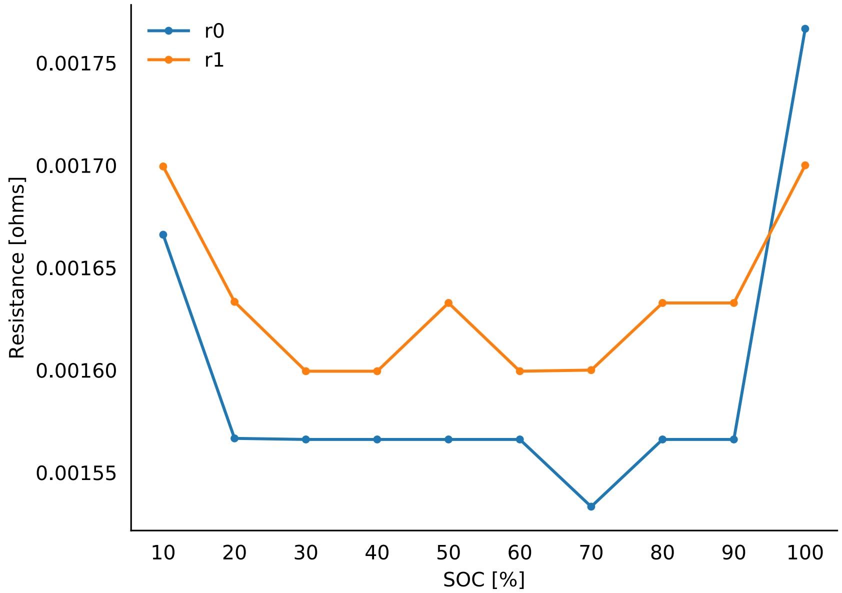
$$v(t) = OCV(z(t)) - R_1\, i_{R_1}(t) - R_0\, i(t)$$

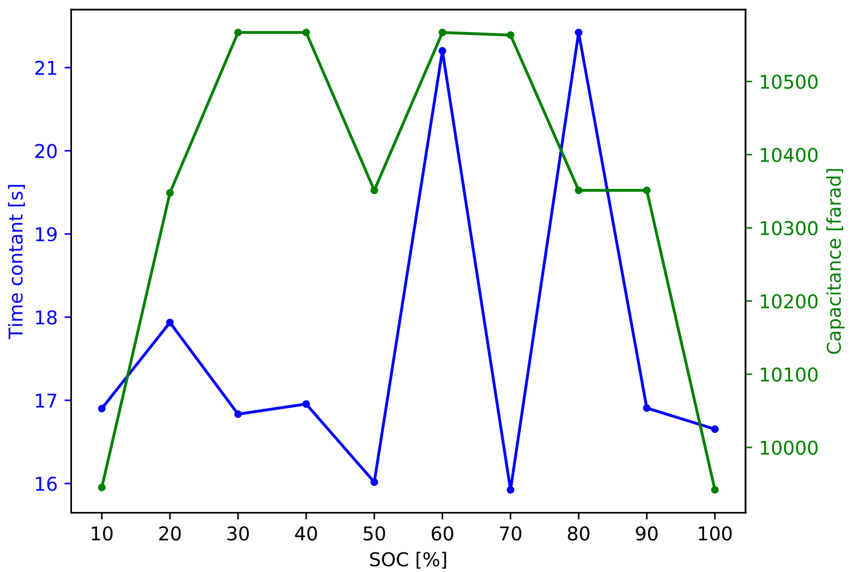


Example of a voltage profile from HPPC test that represents a 10% change in SOC. Equations to determine R-C parameters also shown.

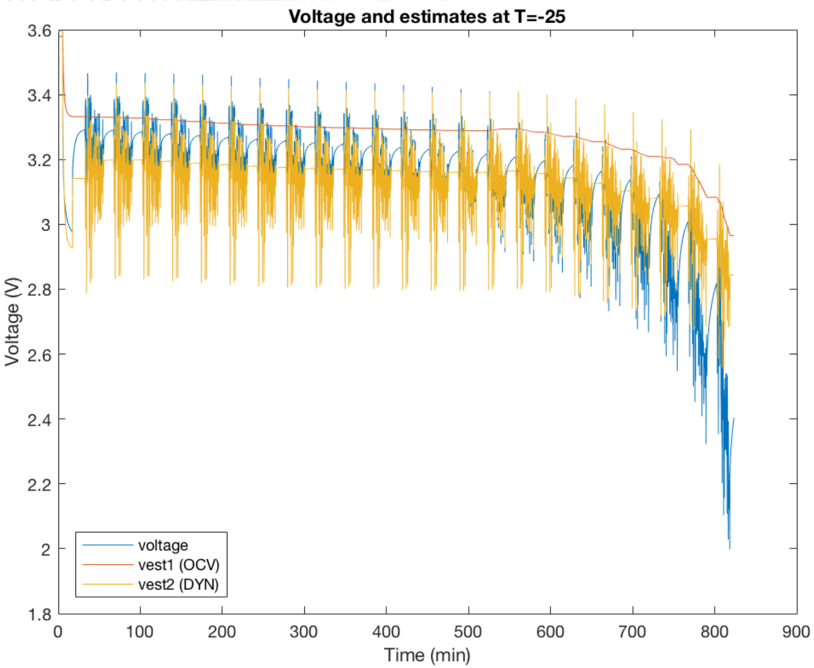
Parameters at each SOC as evaluated from HPPC test

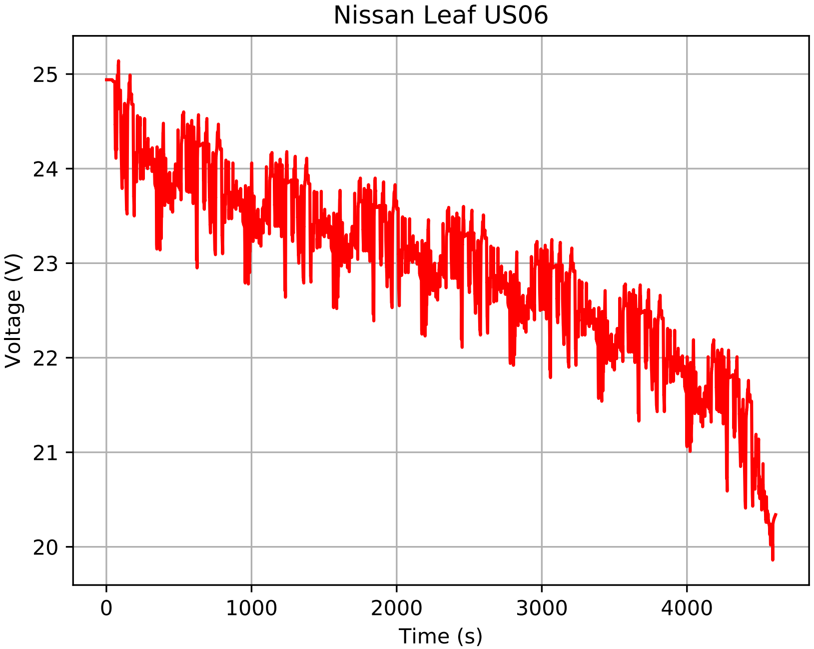
- Parameters are applied to each 10% SOC region
- For example, $R_1 = 0.00164\ \Omega$ for SOC = 80-90%





US06 drive cycle data and SOC for battery module





Comparison of ESC model to actual dynamic voltage profile of a single battery cell at -25°C. Battery data provided by Gregory Plett.

Nissan Leaf voltage profile from US06 drive cycle. Source: NREL 2017.

Goal is to implement reduced order modeling approach to determine behavior of entire battery module.